Emission Properties of Non-equilibrium Zirconium Plasma in Soft X-ray Region

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Marie Curie Action

Emission properties of non-eq Zr plasma

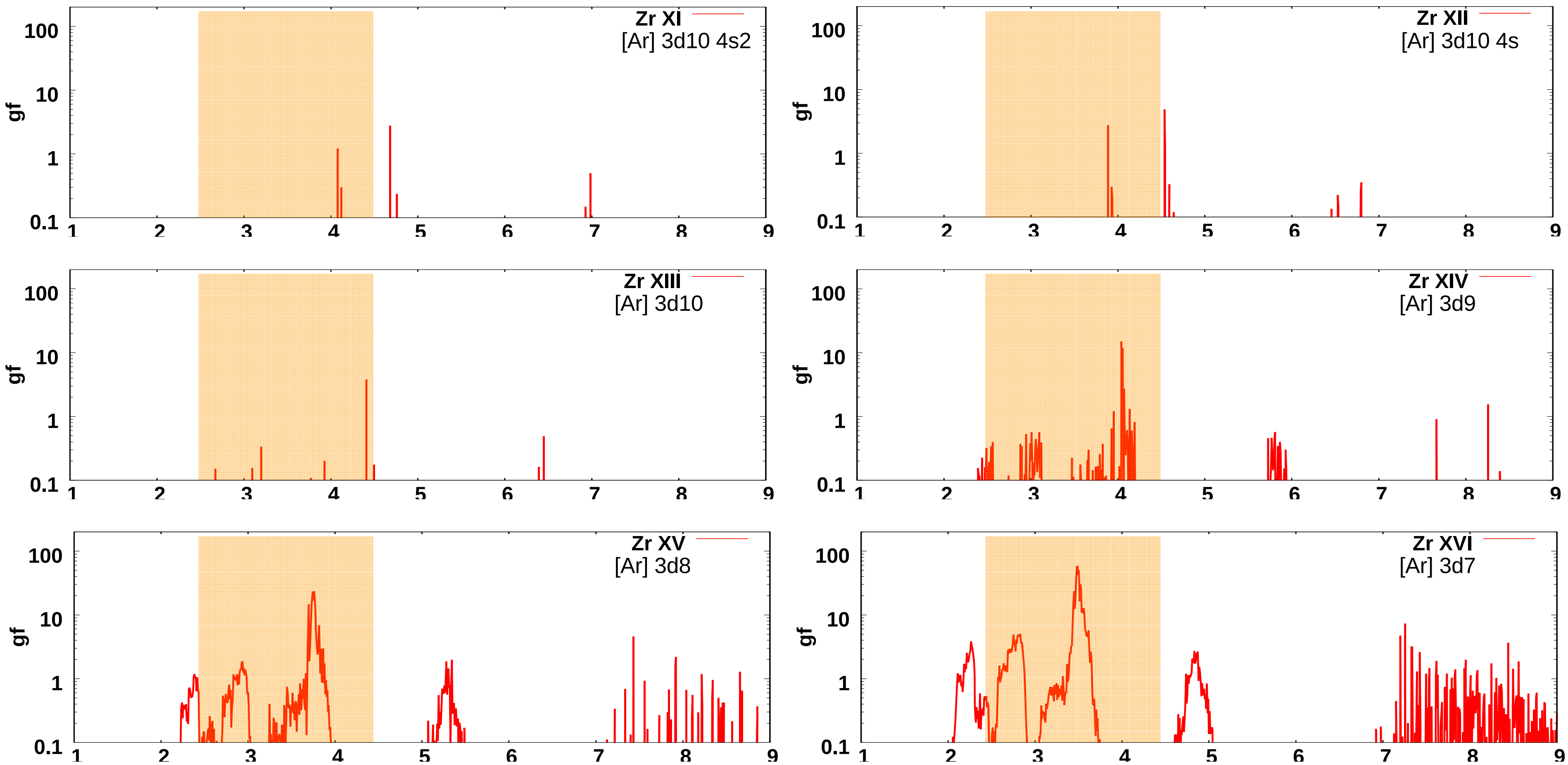
Abstract

Zirconium-based plasmas are considered as a source of soft X-ray emission in water window waveband alongside with nitrogen- and bismuth-based radiation plasma sources. Such discharge and laser produced plasmas used in soft X-ray (and EUV) sources are in non-equilibrium state as a rule. This leads to a mismatch between the actual conditions of the plasma and its theoretical/computational estimations because of different effects like non-thermal electron distribution, self-absorption etc. leading to changes in ionization states, state populations, emission intensity and spectrum. In the report the radiance and emission properties of non-equilibrium zirconium plasma is examined and the optimal emission conditions for soft X-ray emission in water window region are explored. Kinetic parameters for non-equilibrium plasma including major inelastic ion interaction processes with non-thermal electrons and radiation, emission and absorption data are obtained in the approach based on Hartree-Fock-Slater (HFS) quantum-statistical model and distorted waves approximation. Modeling of plasma properties and emission is performed by using atomic, kinetic, radiation transport and RMHD Z* code.

Authors kindly thanks Prof. Gerry O’Sullivan for the idea of current work

Zirconium XI – XVI Lines

Zirconium Line strengths in Water Window region

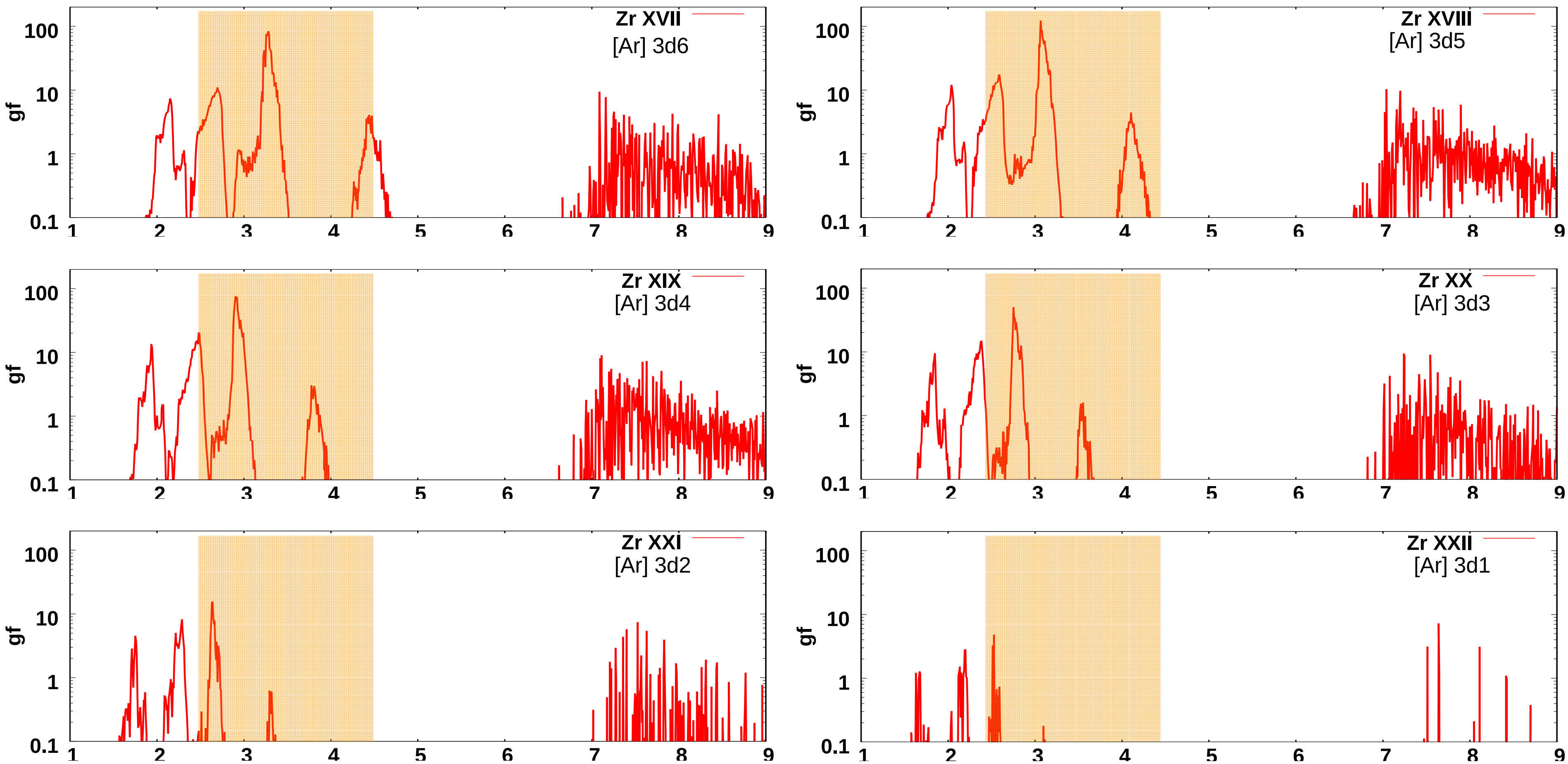


4f-3d, 5p-3d transitions in Zr XI – Zr XX intensively emit in water window (WW) region

Line strengths of Zr XI – Zr XVI computed with Flexible atomic code

Zirconium XVII – XXII Lines

Zirconium Line strengths in Water Window region



Most intensive 4p-3d transitions start to contribute into WW region beginning from Zr XV up to Zr XXI

Line strength of Zr XVI – Zr XXII computed with Flexible atomic code

Non-Equilibrium Model

System of Kinetic equations

To calculate spectrum of emission we need to resolve the system of kinetic equations to obtain relative populations n_μ of levels

$$\frac{dn_\mu}{dt} = \sum_{\nu \neq \mu}^{\nu} n_\nu \alpha_{\nu \to \mu}(N_i, N_e, T, \rho, F) -$$

$$- n_\mu \sum_{\nu \neq \mu}^{\nu} \alpha_{\mu \to \nu}(N_i, N_e, T, \rho, F), \qquad \sum_\mu n_\mu = 1,$$

$\boldsymbol{\alpha_{\nu\to\mu}}$ and $\boldsymbol{\alpha_{\mu\to\nu}}$ - total rates of the processes leading to increase and decrease of the level $\boldsymbol{\mu}$ population $\boldsymbol{n_\mu}$, $\boldsymbol{N_i}$ and $\boldsymbol{N_e}$ – number of ions and electrons, $\boldsymbol{T}$ – temperature, $\boldsymbol{\rho}$ – density. Total rates include a different set of processes depending of model, kind of modelling etc.

Quasi-neutrality:

$$N_e = Z_0 N_i, \qquad Z_0 = \sum_\mu z_\mu n_{\mu},$$

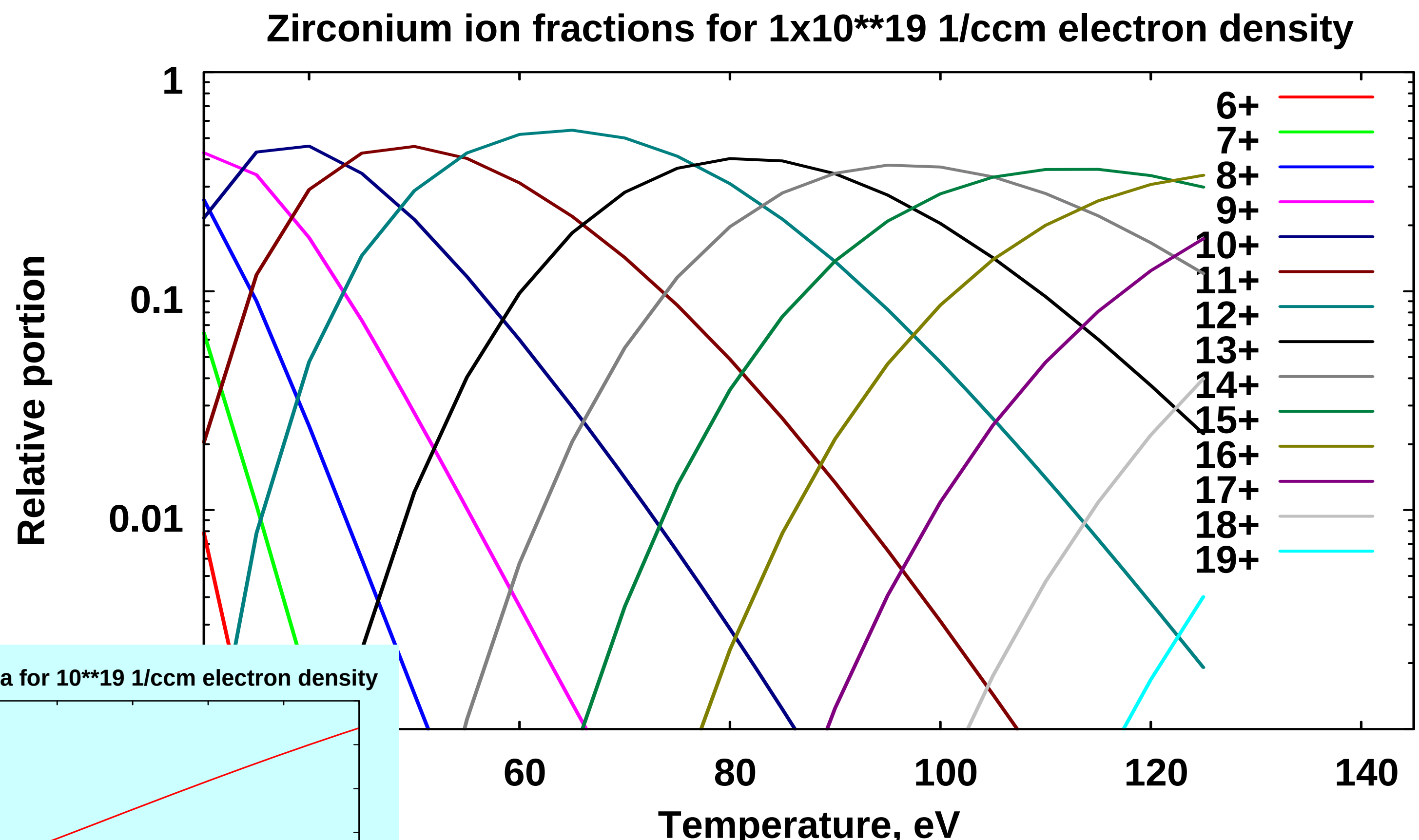
$\boldsymbol{z_\mu}$ – charge of the ion of level $\boldsymbol{\mu}$, $\boldsymbol{Z_0}$ - average charge

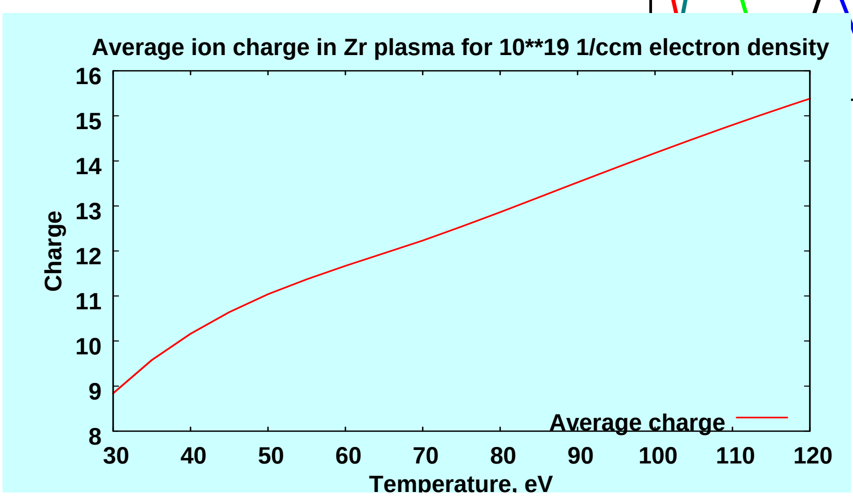
Zirconium Non-equilibrium Plasma

Zirconium Ion populations

Electron density

$N_e = 10^{19}$ 1/ccm

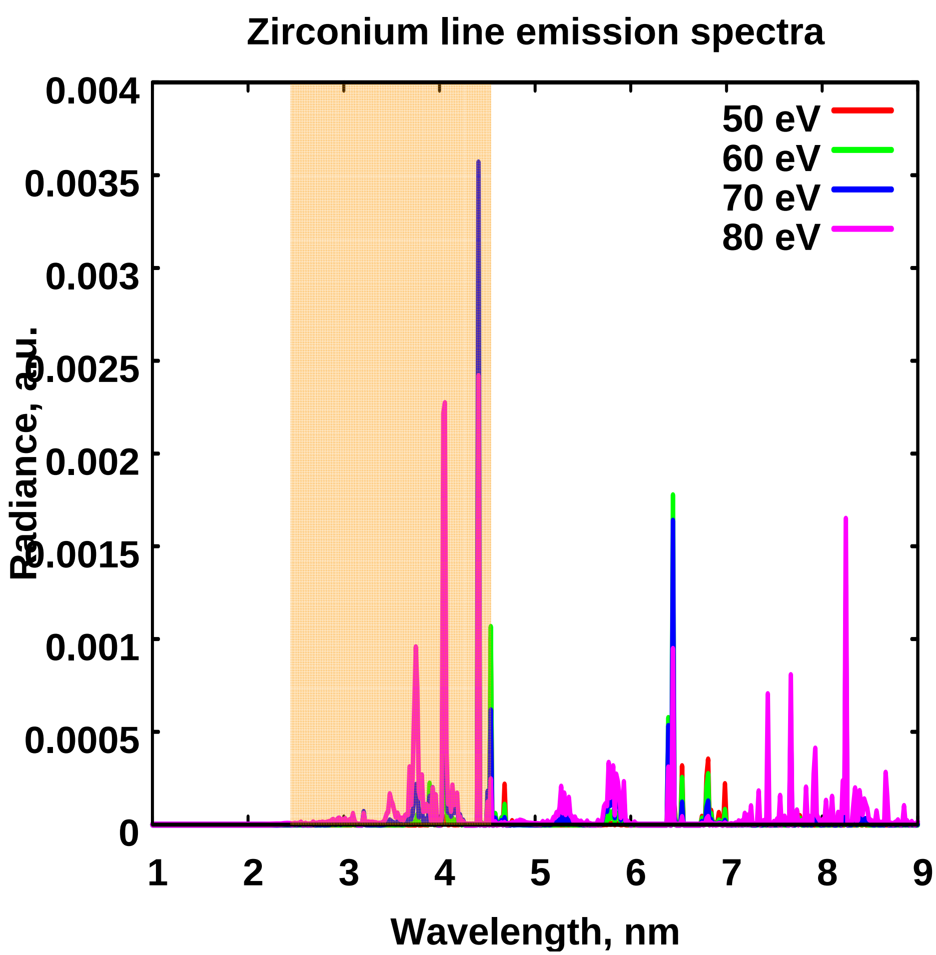


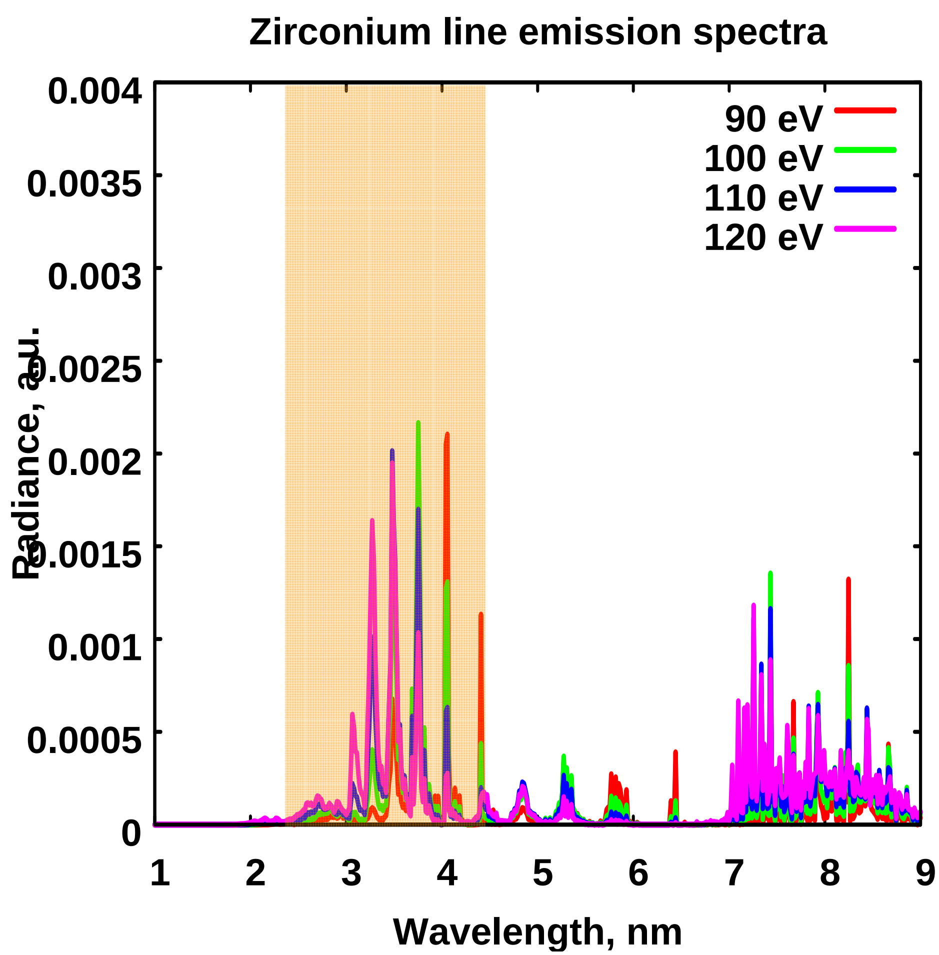


Best conditions for emission in water window are expected at T > 80 eV and higher

Zirconium Plasma Radiance at 50–120 eV

Zirconium Line emission in Water Window region





Spectral Efficiency (SE) reaches its maximum (over 40%) at plasma temperature ~90 eV and decreases slightly after: SE = 2%(50eV) – 33%(70eV) – 40%(90eV) – 38%(110eV)

Radiation transfer in plasma

$$\frac{1}{c}\frac{\partial I_\omega}{\partial t}+(\vec{\Omega}\nabla)I_\omega = j_\omega - k_\omega I_\omega \quad \Rightarrow \quad \frac{\partial I_\omega}{\partial \vec{l}} = j_\omega - k_\omega I_\omega$$ - **Quasi-stationary**

$$U_\omega = c^{-1}\int I_\omega d\vec{\Omega};$$ - **Spectral radiation energy density**

$$\kappa_\omega(n_e,n_i,T_e,U_\omega);$$ - **Opacity**

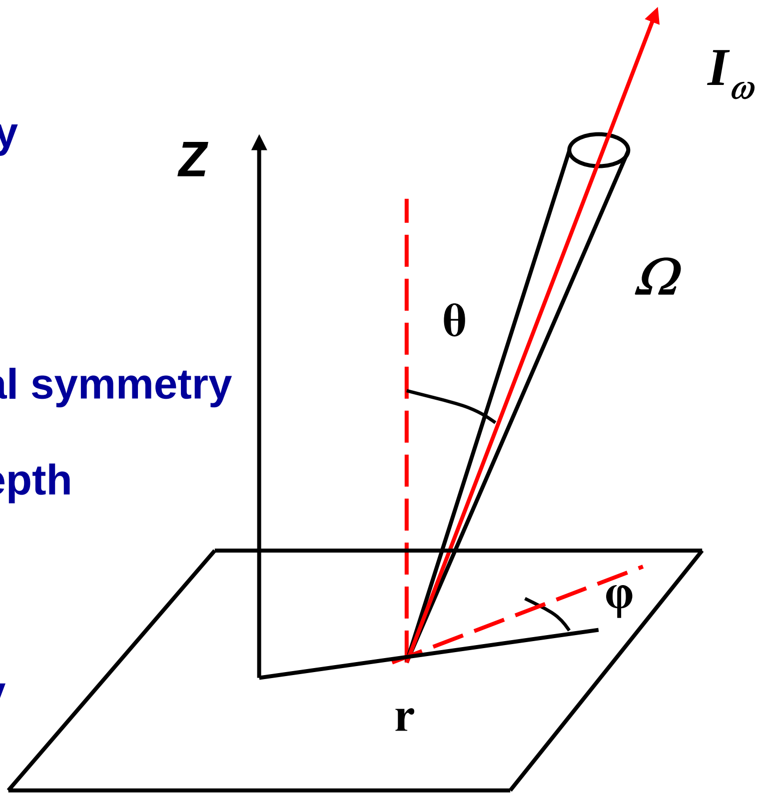
$$j_\omega(n_e,n_i,T_e,U_\omega);$$ - **Emissivity**

$$I_\omega(r,z,\varphi,\theta)=\int_0^\tau \frac{j_\omega}{\kappa_\omega} e^{\tau'-\tau} d\tau;$$ - **Intensity**

- **Cylindrical symmetry**

$$\tau=\tau(x)=\int_0^x \frac{\kappa_\omega(r,z)}{\sin\theta}dx;$$ - **Optical depth**

$$x=\sqrt{r_{out}^2 - r^2\sin^2\varphi}+r\cos\varphi$$
$$z= z_{out}+x\cdot ctg\theta$$ - **Trajectory**



Absorption coefficients

Bound-Bound (bb), Bound-Free (bf) & Free-Free (ff) processes

$$\kappa_\omega = \kappa_\omega^{bb} + \kappa_\omega^{bf} + \kappa_\omega^{ff}$$

$$\kappa_\omega^{bb} = N_i (1 - e^{-\omega/T_e}) \sum_s P_s \sum_{\nu\mu} n_\nu^s \left(1 - n_\mu^s\right) \sigma_{\nu\mu}^{bb}$$

$$\kappa_\omega^{bf} = N_i (1 - e^{-\omega/T_e}) \sum_\nu n_\nu \left(1 - f(\varepsilon)\right) \sigma_{\nu\varepsilon}^{bf}$$

$$\kappa_\omega^{ff} = N_e (1 - e^{-\omega/T_e}) \int d\varepsilon' \, f(\varepsilon') \left(1 - f(\varepsilon)\right) \sigma_{\varepsilon\varepsilon'}^{ff}$$

$$f(\varepsilon) = 1/\left(1 + exp((\varepsilon - \mu)/T)\right)$$

Emissivity

Emissivity in LTE and nonLTE cases

Emissivity (LTE): $$j_\omega = \kappa_\omega I_\omega^p; \qquad I_\omega^p = \frac{\omega^3}{e^{\omega/T} - 1}$$

Emissivity (general nonLTE)

$$j_\omega = j_\omega^{bb} + j_\omega^{fb} + j_\omega^{ff}$$

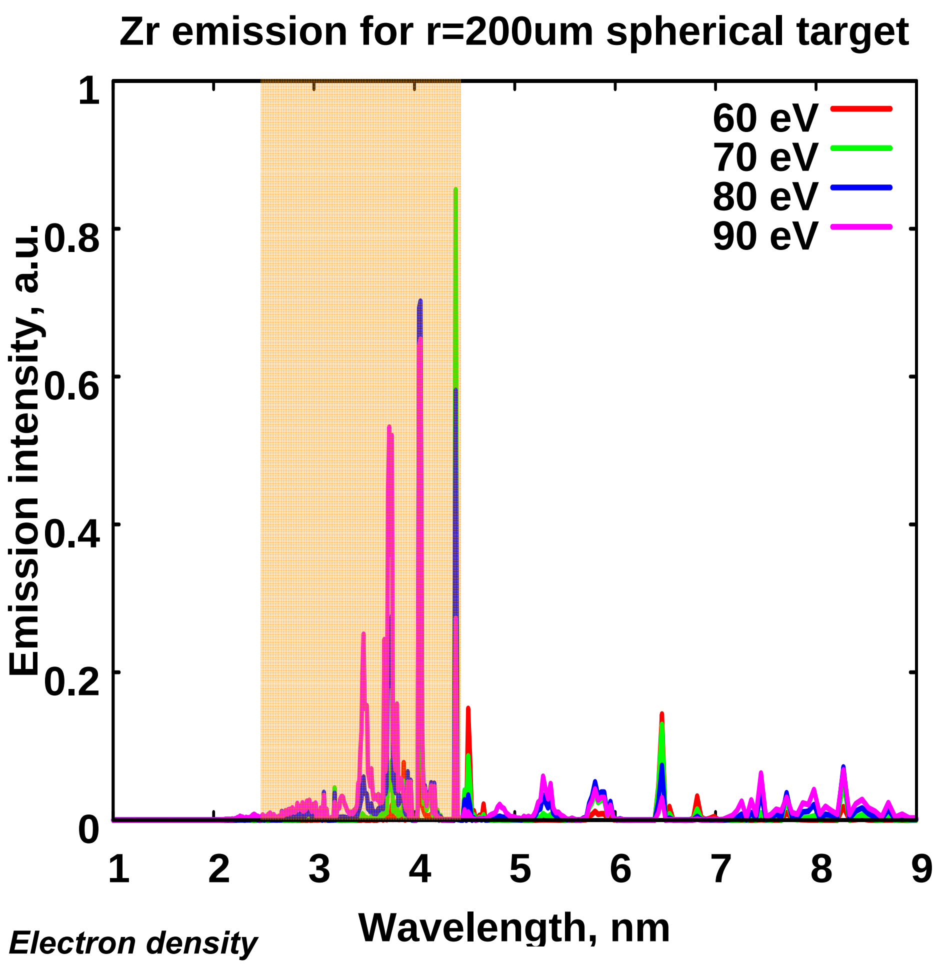
$$j_\omega^{bb} = N_i \omega^3 \sum_s P_s \sum_{\nu\mu} n_\mu^s \left(1 - n_\nu^s\right) \sigma_{\nu\mu}^{bb}$$

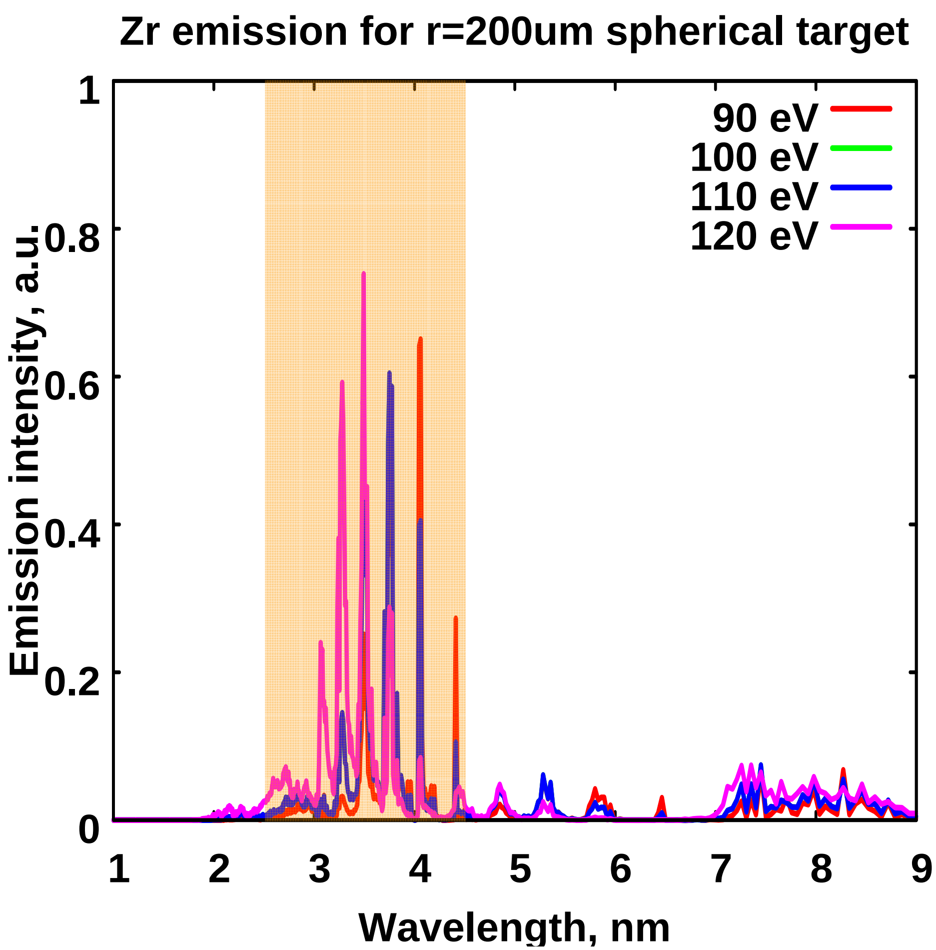
$$j_\omega^{fb} = N_i N_e \omega^3 \sum_\mu f(\varepsilon')\left(1 - n_\mu\right) \sigma_{\nu\varepsilon}^{bf}$$

$$j_\omega^{ff} = N_e N_i \omega^3 \int d\varepsilon\, f(\varepsilon)\left(1 - f(\varepsilon')\right) \sigma_{\varepsilon\varepsilon'}^{ff} \qquad \varepsilon' = \varepsilon + \omega$$

Zirconium target emission

Spectral Modeling for Zirconium spherical target





Electron density

$N_e=10^{19}$ 1/ccm

Spherical target

r = 200 µm

Temperature raises → Broadening → Power of emission

Efficiency?

Remarks

- Zirconium ions XV – XXI emit intensively in water window region: 4p-3d, 4f-3d and 5p-3d transitions

- Maximum spectral efficiency for emission in water window region is over 40% for plasma at temperature of 80eV and hotter

- For spherical target of 200um radius and 10^{19} electron density the spectrum is broadened (absorption broadening)

The results were obtained in frame of FP7 FIRE Marie Curie action

fire

Fluid, Ions and Radiation Ensemble in Integrated Plasma Modelling